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Title: Proposal, Precompound Emission of Energetic Light Fragments in Spallation Reactions

Author(s): Kerby, Leslie M.

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PRECOMPOUND EMISSION OF ENERGETIC LIGHT FRAGMENTS IN SPALLATION REACTIONS

A Proposal

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Degree of Doctorate of Philosophy

with a

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by

Leslie M. Kerby

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Major Professor: Akira T. Tokuhiro, Ph.D.

Los Alamos National Laboratory Mentor: Stepan G. Mashnik, Ph.D.

Ruprecht Machleidt, Ph.D.

Francesca Sammarruca, Ph.D.

Forrest B. Brown, Ph.D

Table of Contents

1 Introduction

Emission of light fragments (LF) from nuclear reactions is an open question because different reaction mechanisms contribute to their production, and the relative roles of each, and how they change with incident energy, mass number of the target, and the type and emission energy of the fragments is not completely understood.

None of the available models are able to accurately predict emission of LF from arbitrary reactions. However, the ability to describe production of LF (especially at energies $\gtrsim$ 30 MeV) from many reactions is important for different applications, such as cosmic-ray-induced Single Event Upsets (SEUs), radiation protection, and cancer therapy with proton and heavy-ion beams, to name just a few. The Cascade-Exciton Model (CEM) [1] version 03.03 and the Los Alamos version of the Quark-Gluon String Model (LAQGSM) [2, 3] version 03.03 event generators in Monte Carlo N-Particle Transport Code version 6 (MCNP6) [4] describe well the spectra of fragments with sizes up to ^{4}He across a broad range of target masses and incident energies (up to $\sim$ 5 GeV for CEM and up to $\sim$ 1 TeV/A for LAQGSM). However, they do not predict the high-energy tails of LF spectra heavier than ^{4}He well because most LF with energies above several tens of MeV are emitted during the precompound stage of a reaction, and the current versions of the CEM and LAQGSM event generators do not account for precompound emission of LF larger than ^{4}He.

The aim of our work is to extend the precompound model in them to include emission of light fragments up to ^{28}Mg, leading to an increase of predictive power of LF-production in MCNP6. This entails upgrading the Modified Exciton Model currently used at the preequilibrium stage in CEM and LAQGSM. It will also include investigation and possible expansion of the coalescence and Fermi break-up models used in the precompound stages of spallation reactions within CEM and LAQGSM. Extending our models to include emission of fragments heavier than ^{4}He at the precompound stage has already provided preliminary results that have much better agreement with experimental data.

2 Why This Research Is Important

In October 2008 an Airbus plane was struck by a cosmic ray en route from Perth to Singapore, one of its inertial reference computer units failed, and it sharply lost altitude [5]. It did land safely, but as seen in Figure 1, it caused significant injury to both the occupants and the plane.

Figure 1: Photographs of the damaged Airbus after the SEU [5].

These SEUs are not rare, and can wreak significant havoc. For example, in a typical 14-day space mission the shuttles' 5 computers typically receive 400-500 SEUs [6]. In addition, even though the plane accident was serious, much more serious incidents have occurred: during the Cold War, computer chips have failed and incorrectly shown missile launches, creating false alarms.[7]. SEUs can cause failures like this in satellites. Understanding how high-energy fragments interact with matter is critical to preventing these malfunctions.

Accurate simulation of LF spectra is also important in the fields of radiation shielding, especially for applications in space. Modern computers cannot be used in space because the electronics are too small and delicate and cannot, at present, be shielded well enough. An even larger problem is radiation shielding for the human astronauts exposed to Galactic Cosmic Rays (GCRs) [6].

This research is also important to several medical fields. Most notable is its application to cancer treatment with proton or heavy-ion beams, such as are utilized at the Gunma University Heavy-Ion Medical Center in Maebashi, Japan. Proton and heavy-ion therapy has been shown to be more effective than x-ray therapy, and have much fewer side effects [8].

Another indication of the importance of this research is the recommendation of an international evaluation and comparison, the 2008-2010 IAEA (International Atomic Energy Agency) Benchmark of Spallation Models, that we make this change in our code [9, 10]. While no other spallation model can generally predict high-energy light fragment emission from arbitrary reactions, it is an accomplishment several model development groups are working to achieve.

Furthermore, MCNP6's GENXS option at present does not produce tallies for particles larger than ^{4}He. This limitation is serious for some of our interest groups. For example, NASA recently contacted one of us (SGM) to inquire if our codes could produce LF spectra in the intermediate- and high-energy regimes. At present they cannot.

Last, but not least, this research helps us understand better the mechanisms of nuclear reactions.

3 Precompound Emission of Light Fragments in Other Models

This paper focuses on the emission of high-energy LF at the preequilibrium stage of nuclear reactions. However, high-energy LF can be produced at other stages of reactions. Cugnon *et al.* have modified their Liège IntraNuclear Cascade (INCL) code to consider emission of light fragments heavier than ^{4}He during the cascade stage of reactions via coalescence of several nucleons at the nuclear periphery [11]. These modifications have not yet been generalized across all types of reactions. In addition, the INCL+ABLA model is limited to relatively light incident projectiles (particles and light ions, typically, up to oxygen). Several previous papers by the same group discuss the production of light fragments up to $A = 10$ (see, e.g., [12, 13]). A recent 2013 paper by the same authors presents satisfactory results for emission spectra of ^{6}He, ^{6}Li, ^{7}Li, and ^{7}Be in the reaction $p+^{197}Au \rightarrow ...$ and discusses emission of clusters up to $A = 12$ [14].

Emission of ^{7}Be at the preequilibrium stage (described by a hybrid exciton model and coalescence pick-up model) was studied by A. Y. Konobeyev and Y. A. Korovin more than a decade ago [15]. Additionally, preequilibrium emission of helium and lithium ions and the necessary adjustments to the Kalbach systematics was discussed in Ref. [16]. Preequilibrium emission of light fragments was also studied within the CEM in 2002 [17], but that project was never completed.

Finally, energetic fragments can be produced via Fermi break-up [18] and multifragmentation processes, as described, e.g., by the Statistical Multifragmentation Model (SMM) [19]; (see a comparison of the Fermi break-up model with SMM in the recent paper by Souza *et al.* [20]).

Light fragments can also be emitted during the compound stage of reactions. GEM2, the evaporation model used in CEM, emits light fragments up to ^{28}Mg [21]. In addition, light fragments can be produced via very asymmetric binary fission, as described, e.g., by the fission-like binary decay code GEMINI by Charity et al. [22], and also via ternary fission. For more information, see the recent Ref. [23] wherein Y. Ronen discusses the physics of how light fragments are products seen in ternary fission. However, neither evaporation nor fission processes can produce high-energy fragments, of interest to our current study.

4 Statement of Project

This project involves expanding the precompound models within CEM to more accurately describe energetic LF spectra. There are several aspects of this project:

1. Modify CEM code to emit 66 particles (vs 6 originally) in the preequilibrium modules;
2. Parameterize γ_β for ~ 100 proton spallation reactions;
3. Parameterize γ_β for ~ 50 neutron spallation reactions;
4. Analyze γ_β parameterization for a possible physical/mathematical model;
5. Re-write γ_β CEM modules to either incorporate the new mathematical model or utilize modern interpolation and extrapolation methods using our parameterization;
6. Investigate Fermi break-up model expansion;
7. Investigate coalescence model expansion;
8. Replace the MEM in LAQGSM with our expanded MEM and test;
9. Extend GENXS option of MCNP6 to allow emission of LF and test;
10. Replace upgraded CEM and LAQGSM modules in MCNP6 and test.

Item 1 has been completed. Items 2 and 6 have been partially completed. Figure 2 demonstrates the potential of the modified precompound code we built for the reaction 190 MeV p + ^{nat}Ag. The red solid lines show results from the new precompound code we designed in FY2013; the blue dotted lines present calculations from the old code; and the green points are experimental data from Green, *et al.* [24]. The upgraded MEM provides dramatically improved ability to describe the cross section at intermediate to high energies.

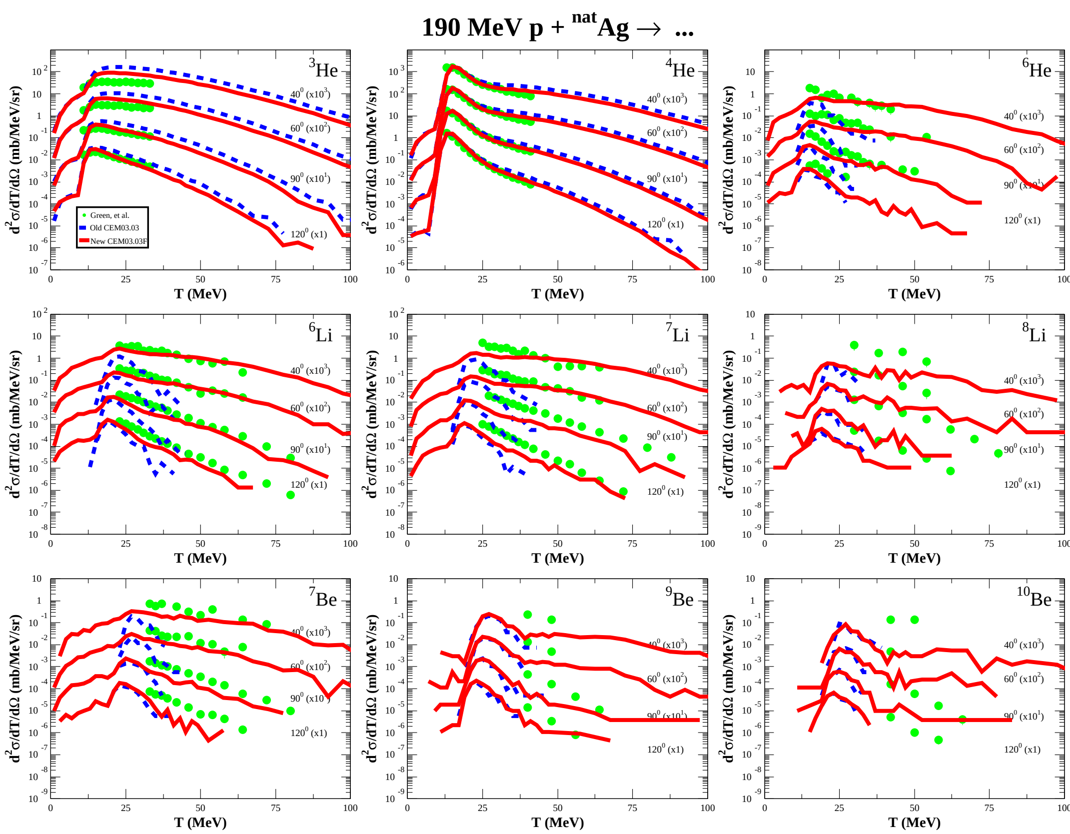

Figure 2: Comparison of experimental data by Green *et al.* [24] (green points) with results from the unmodified CEM03.03 (blue dotted lines) and the modified MEM CEM03.03 (red solid lines) for 190 MeV p + ^{nat}Ag → ...

So far, presentations have been made at ND2013 and INPC2013 on this research and will appear in Nuclear Data Sheet and European Physical Journal Web of Conferences. Future presentations will be given and at least two publications will be submitted to major peer-reviewed journals, such as Nuclear Physics A and Physical Review C.

5 Explanation of Limitations

1. We will not investigate modifications to the evaporation model used in CEM (GEM2). This was last investigated as a Ph.D. dissertation by Furihata [21] and is a massive project all by itself;

2. We will not consider reactions induced by pions or other particles besides protons and neutrons. Proton- and neutron-induced reactions are of most interest to LANL;

3. Where possible, new code will be written in Fortran 90; but the bulk of the CEM code will remain in Fortran 77;

4. The availability of experimental data for the emission of energetic LF from various targets and energies is not abundant; therefore our parameterization of γ_β for some emitted light fragments will be based on few experimental results.

6 Tools and Skillset Required

1. Knowledge of Spallation Reactions. A thorough understanding of the stages and modeling of spallation reactions, both within the CEM model and in other competing models, is essential to this work. I am familiar with these models, but greater depth is desirable. Further study of "Handbook of Spallation Research" by D. Filges and F. Goldenbaum is recommended.

2. Fortran Programming Capability. Profienciency in both Fortran 77 and Fortran 90 is required for this research so that I can understand the current CEM codes but write new modules according to accepted guidelines used presently in MCNP6. I have these skills presently.

3. Physics Analysis Workstation Profiency. PAW is being used to produce the hundreds of graphs necessary to parameterize γ_β. It will also be used to analyze these parameterizations to glean a possible mathematical model. While I have learned PAW and use it currently in my work, I still need to learn the specifics of using PAW to numerically analyze this data, and will learn this from internet tutorials. I will also consult with Ruprecht Machleidt and Francesca Sammarruca on mathematical modeling methods.

4. Numerical Interpolation and Extrapolation Methods. As part of my work I will entirely re-write the interpolation and extrapolation routines for γ_β. I will consult with Forrest Brown on efficient and effective numerical methods to accomplish this.

5. Familiarity with CEM and LAQGSM codes. I am currently familiar with CEM, but will need to also become familiar with LAQGSM to implement improvements in that code as well. Stepan Mashnik and Arnold Sierk will teach me LAQGSM.

6. MCNP6 Modification Procedures. The final step of this research will be modifying the GENXS option within MCNP6 and implementing our improvements in MCNP6. Stepan Mashnik, Forrest Brown, and Larry Cox will guide me on where in the code these changes need to be made, and how to make these changes according to XCP-3 code modification procedures.

7 Timeline

An approximate timeline is provided in Table 1.

Table 1: Timeline

	2014				2015				2016			
	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4
Proton-induced reactions		X										
Neutron-induced reactions			X									
γ_β model analysis				X								
γ_β code modifications						X						
Fermi break-up						X						
Coalescence							X					
LAQGSM							X					
GENXS								X				
MCNP6									X			
Dissertation Defense										X		

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